Phase Command-Line Database Management and Searching

Database management tasks can be run in the foreground or submitted as a single-CPU job to any host that has access to the database directory. Site creation and database search jobs can be run on multiple processors. When you create the database, make sure that it is on a file system that is accessible to all hosts that need access to the database. For details on the commands and options, see Chapter 13 of the *Phase User Manual*.

To create a new database:

```
$SCHRODINGER/utilities/phasedb_manage -new dbFileType [-fd fdFile] -db dbname {-mae maeFile|
    -sd sdFile} -confs multiConfs [-ignoreTitles] [job-options]
```

To add molecules to an existing database:

```
$SCHRODINGER/utilities/phasedb_manage -add -db dbname {-mae maeFile|-sd sdFile} -confs multiConfs
    [-ignoreTitles] [job-options]
```

To delete molecules from a database:

```
$SCHRODINGER/utilities/phasedb_manage -delete -db dbname -records recordFile [job-options]
```

To create a subset from the structures in a hit file:

```
$SCHRODINGER/utilities/phasedb_subset -db database -hits hitfile -out subset
```

To create a subset from a logical operation on two existing subsets:

```
$SCHRODINGER/utilities/phasedb_subset -db database -in1 subset1 -logic {AND|OR|NOT} -in2 subset2
    -out subset
```

To create a subset from a query of the database:

```
$SCHRODINGER/utilities/phasedb_subset -db database {-confs|-sites} {true|false} -out subset
```

To competely remove a database:

```
$SCHRODINGER/utilities/phasedb_manage -delete -db dbname -all [job-options]
```

To generate conformers and pharmacophore sites:

```
$SCHRODINGER/utilities/phasedb_confsites -db dbname [-sub dbSubset] -JOB jobname [job-options]
     [-confs {auto|all} [-sample {rapid|thorough}] [-max maxConfs] [-ewin deltaE] ]
```

To convert a database:

```
$SCHRODINGER/utilities/phasedb_convert -source dbSource -target dbTarget [-new {sd|mae}]
    [-fd fdFile] [-records recordFile] [-restart] [-final] [-delete]
```

To search for matches in a database:

```
$SCHRODINGER/utilities/phasedb_findmatches -setup jobname -db dbName -hypo hypoID -mode runMode
    [-sub dbSubset] [-dtol deltaDist] [-minSites minSites] [-matchFile matchFile] [-maxHits maxHits]
```

```
$SCHRODINGER/phase_dbsearch [job-options] [-BLOCK m] jobname
```

```
$SCHRODINGER/utilities/phasedb_findmatches -cleanup jobname
```

In the commands above, *job-options* represents the standard Job Control options:

`-HOST` *host*	Run the job on the specified host.
`-LOCAL`	Run the job in the current directory, rather than in a temporary scratch directory.
`-TMPDIR` *tmpdir*	Use *tmpdir* for temporary files.
`-WAIT`	Do not return control to the shell until the job finishes.
`-INTERVAL` *n*	Interval in seconds between output updates.
`-NICE`	Run the job at reduced priority.